Multiparameter exponentially-fitted methods applied to second-order boundary value problems

M. Van Daele, D. Hollevoet and G. Vanden Berghe

Vakgroep Toegepaste Wiskunde en Informatica, Ghent University, Krijgslaan 281-S9, B9000 Gent, Belgium

Abstract. Second-order boundary value problems are solved by means of a new type of exponentially-fitted methods that are modifications of the Numerov method. These methods depend upon a set of parameters which can be tuned to solve the problem at hand more accurately. Their values can be fixed over the entire integration interval, but they can also be determined locally from the local truncation error. A numerical example is given to illustrate the ideas.

Keywords: Boundary value problems; second-order problems; Numerov method; Exponential fitting
PACS: 02.60.Lj

INTRODUCTION

The Numerov method, given by

$$y_{j-1}-2y_j+y_{j+1}=\frac{h^2}{12}\left(y''_{j-1}+10y''_j+y''_{j+1}\right), \tag{1}$$

is a well-known fourth-order method for solving second-order boundary value problems of the form

$$y''=f(t,y), \qquad y(a)=\alpha, \qquad y(b)=\beta,$$

whereby, for simplicity, we assume that y and f are real. To do so, one first applies Eq. (1) at a number of equidistant points $t_j := a+jh$, $j=1,\ldots,N$ where $h:=(b-a)/(N+1)$ and secondly a (possibly nonlinear) system has to be solved. In recent papers [4, 5], we constructed so-called exponentially fitted (EF) versions of this method by imposing six conditions related to the members of the fitting space

$$\mathscr{S}_{K,P}(\mu)=\{1,t,t^2,\ldots,t^K\}\cup\{\exp(\pm\mu t),t\exp(\pm\mu t),\ldots,t^P\exp(\pm\mu t)\}$$

where $P\in\{-1,0,1,2\}$ and $K=3-2P$, on the linear difference operator $\mathscr{L}[h,\mathbf{a}]$. This operator is defined as

$$\mathscr{L}[h,\mathbf{a}]y(t):=y(t-h)+a_0y(t)+y(t+h)-h^2\left(b_1y''(t-h)+b_0y''(t)+b_1y''(t+h)\right). \tag{2}$$

For $P=-1$, the classical Numerov method is obtained. For $P\in\{0,1,2\}$, an EF method arises. An important issue w.r.t. the application of such an EF method is the way in which its parameter μ is determined. In [4, 5] this parameter was determined starting from the expression for the local truncation error (lte) of the resulting method. This lte, as a function of $Z:=(\mu h)^2$, takes the form (for $|Z|$ sufficiently small a closed expression can be written down, see [2, 3, 5])

$$h^6\,\phi_P(Z)\,D^{K+1}\,(D^2-\mu^2)^{P+1}\,y(t_j)+\mathscr{O}(h^8),$$

where $\phi_P(Z)=-\frac{1}{240}+\mathscr{O}(Z)$. At each point t_j, a value μ_j^2 for μ^2 is then computed such that

$$D^{K+1}\,(D^2-\mu_j^2)^{P+1}\,y(t_j)=0\,.$$

For $P=0$, this always leads to $\mu_j^2\in\mathbb{R}$. For $P=1$ however, it may happen that both roots μ_j^2 of

$$y^{(6)}(t_j)-2\mu^2y^{(4)}(t_j)+\mu^4y^{(2)}(t_j)=0$$

are complex. In that case, the numerical solution obtained with this method will be complex. To solve this problem, we propose a new type of EF methods.

DERIVATION OF THE METHODS

We start from the fitting space

$$\widehat{\mathscr{S}_{K,P}}(\mu_0,\mu_1,\ldots,\mu_P) = \{1,t,t^2,\ldots,t^K\} \cup \{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), \ldots, \exp(\pm\mu_P t)\}\,,$$

where the parameters μ_q, $q=0,\ldots,P$ are either real or appear as complex conjugate pairs. In order to obtain expressions for the coefficients a_0, b_0 and b_1 of the method, we impose for each member $y(t)$ of this set the condition (2). Denoting $Z_q := (\mu_q h)^2$, $\xi_q := \xi(Z_q)$ and $\eta_q := \eta(Z_q)$, where ξ and η are defined (see [1], p. 64) as

$$\xi(Z) = \cos(i\sqrt{Z}) \qquad \text{and} \qquad \eta(Z) = \begin{cases} \dfrac{\sin(i\sqrt{Z})}{i\sqrt{Z}} & \text{if } Z \neq 0 \\ 1 & \text{if } Z = 0\,, \end{cases}$$

we obtain the following expressions

(i) $P=-1$:

$$a_0 = -2 \qquad b_0 = \frac{5}{6} \qquad b_1 = \frac{1}{12}\,.$$

(ii) $P=0$:

$$a_0 = -2 \qquad b_0 = \frac{-2\,\xi_0 + 2 + \xi_0 Z_0}{Z_0\,(\xi_0 - 1)} \qquad b_1 = -\frac{1}{2}\,\frac{Z_0 - 2\,\xi_0 + 2}{Z_0\,(\xi_0 - 1)}\,.$$

(iii) $P=1$:

$$a_0 = -2 \qquad b_0 = -2\,\frac{\xi_0\,(\xi_1 - 1)\,Z_0 + \xi_1\,(1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)} \qquad b_1 = \frac{(\xi_1 - 1)\,Z_0 + (1-\xi_0)\,Z_1}{Z_1 Z_0\,(\xi_1 - \xi_0)}\,.$$

In the special case where $Z_1 \to Z_0$ we have

$$\lim_{Z_1\to Z_0} b_0 = \frac{4\,{\xi_0}^2 - 4\,\xi_0 - 2\,\eta_0 Z_0}{{Z_0}^2 \eta_0} \qquad \lim_{Z_1\to Z_0} b_1 = \frac{\eta_0 Z_0 + 2 - 2\,\xi_0}{{Z_0}^2 \eta_0}\,.$$

These are exactly the coefficients which are obtained for the fitting space $\mathscr{S}_{1,1}(\mu_0) = \{1,\, t,\, \exp(\pm\mu_0 t),\, t\,\exp(\pm\mu_0 t)\}$. In fact, this just illustrates the general property

$$\lim_{\mu_1\to\mu_0} \widehat{\mathscr{S}_{K,1}}(\mu_0,\mu_1) = \mathscr{S}_{K,1}(\mu_0)\,.$$

(iv) $P=2$:

$$\begin{aligned}
a_0 &= -2\,\frac{(-\xi_0\,(\xi_1-\xi_2)\,Z_2 + \xi_2\,(-\xi_0+\xi_1)\,Z_0)\,Z_1 + \xi_1\,(\xi_0-\xi_2)\,Z_0 Z_2}{(\xi_2-\xi_1)\,Z_1 Z_2 + (\xi_1-\xi_0)\,Z_0 Z_1 + (\xi_0-\xi_2)\,Z_0 Z_2} \\
b_0 &= -2\,\frac{-\xi_1\,(\xi_0-\xi_2)\,Z_1 - \xi_2\,(-\xi_0+\xi_1)\,Z_2 + \xi_0\,(\xi_1-\xi_2)\,Z_0}{(\xi_2-\xi_1)\,Z_1 Z_2 + (\xi_1-\xi_0)\,Z_0 Z_1 + (\xi_0-\xi_2)\,Z_0 Z_2} \\
b_1 &= \frac{(-\xi_0+\xi_2)\,Z_1 + (\xi_0-\xi_1)\,Z_2 + (\xi_1-\xi_2)\,Z_0}{(\xi_2-\xi_1)\,Z_1 Z_2 + (\xi_1-\xi_0)\,Z_0 Z_1 + (\xi_0-\xi_2)\,Z_0 Z_2}\,.
\end{aligned}$$

Again we can consider some special cases. A first one is obtained when $Z_2 \to Z_1$:

$$\begin{aligned}
\lim_{Z_2\to Z_1} a_0 &= -2\,\frac{2\,Z_0 {\xi_1}^2 - 2\,\xi_1 \xi_0 Z_0 + \xi_0 Z_1\,(Z_0 - Z_1)\,\eta_1}{2\,Z_0 \xi_1 + Z_1\,(Z_0 - Z_1)\,\eta_1 - 2\,\xi_0 Z_0} \\
\lim_{Z_2\to Z_1} b_0 &= -2\,\frac{2\,{\xi_1}^2 - 2\,\xi_1 \xi_0 + \xi_0\,(Z_0 - Z_1)\,\eta_1}{2\,Z_0 \xi_1 + Z_1\,(Z_0 - Z_1)\,\eta_1 - 2\,\xi_0 Z_0} \\
\lim_{Z_2\to Z_1} b_1 &= \frac{2\,\xi_1 + (Z_0 - Z_1)\,\eta_1 - 2\,\xi_0}{2\,Z_0 \xi_1 + Z_1\,(Z_0 - Z_1)\,\eta_1 - 2\,\xi_0 Z_0}\,.
\end{aligned}$$

These are the coefficients that are obtained for the fitting space $\{\exp(\pm\mu_0 t), \exp(\pm\mu_1 t), t\exp(\pm\mu_1 t)\}$. In the particular case where both Z_2 and Z_1 tend to Z_0, we obtain

$$\begin{aligned}
\lim_{\substack{Z_1\to Z_0\\ Z_2\to Z_0}} a_0 &= 2\,\frac{{\xi_0}^2-2-3\,\eta_0\xi_0}{\xi_0+3\,\eta_0}\\
\lim_{\substack{Z_1\to Z_0\\ Z_2\to Z_0}} b_0 &= 2\,\frac{\eta_0\xi_0+{\xi_0}^2-2}{Z_0\,(\xi_0+3\,\eta_0)}\\
\lim_{\substack{Z_1\to Z_0\\ Z_2\to Z_0}} b_1 &= \frac{\xi_0-\eta_0}{Z_0\,(\xi_0+3\,\eta_0)}\,.
\end{aligned}$$

These are exactly the formulae that are obtained for the coefficients when the fitting space $\mathscr{S}_{-1,2}(\mu_0) = \{\exp(\pm\mu_0 t), t\exp(\pm\mu_0 t), t^2\exp(\pm\mu_0 t)\}$ is considered. In fact, this illustrates the general property

$$\lim_{\substack{\mu_1\to\mu_0\\ \mu_2\to\mu_0}} \widehat{\mathscr{S}_{K,2}}(\mu_0,\mu_1,\mu_2) = \mathscr{S}_{K,2}(\mu_0)\,.$$

The expressions for the coefficients given above can only be used when all of the Z_q are mutually well separated and not too close to zero. In such cases, Taylor series approximations need to be used.

SELECTING VALUES FOR THE PARAMETERS

To select appropriate values for the parameters, one can try to annihilate the leading term of the lte, which is now given by

$$h^6\,\widehat{\phi}_P(Z_0,\ldots,Z_P)\,D^{K+1}\,(D^2-\mu_0^2)\,(D^2-\mu_1^2)\cdots(D^2-\mu_P^2)\,y(t_j)+\mathscr{O}(h^8)\,,$$

for some function $\widehat{\phi}_P$ with $\widehat{\phi}_P(Z_0,\ldots,Z_P) = -\frac{1}{240}+\mathscr{O}(Z_0,Z_1,\ldots,Z_P)$. In particular, this means that we will have to annihilate the following expressions :

(i) $P=0: E_{0,j} := y^{(6)}(t_j)-\mu_0^2\,y^{(4)}(t_j)$

(ii) $P=1: E_{1,j} := y^{(6)}(t_j)-(\mu_0^2+\mu_1^2)\,y^{(4)}(t_j)+\mu_0^2\,\mu_1^2\,y^{(2)}(t_j)$

(iii) $P=2: E_{2,j} := y^{(6)}(t_j)-(\mu_0^2+\mu_1^2+\mu_2^2)\,y^{(4)}(t_j)+(\mu_0^2\,\mu_1^2+\mu_0^2\,\mu_2^2+\mu_1^2\,\mu_2^2)\,y^{(2)}(t_j)-\mu_0^2\,\mu_1^2\,\mu_2^2\,y(t_j)$.

For $P=0$, $E_{0,j}=0$ gives a unique way to fix the value of μ_0^2 at the point t_j. For $P=1$ however, we need to fix two parameters μ_0^2 and μ_1^2, so two equations are needed. One of the many possibilities might be to take $E_{1,j}=0=E_{1,j+1}$. In a similar way, for the case $P=2$, the three parameters μ_0^2, μ_1^2 and μ_2^2 can be determined from $E_{2,j-1}=0$, $E_{2,j}=0$ and $E_{2,j+1}=0$.

It should be noted that instead of using variable parameters, one may also use parameters that are constant over the entire integration interval. For instance, for $P=0$ one could use some averaged value μ_0^2 that is obtained from solving (some of) the equations $E_{0,j}=0,\ j=1,\ldots,N$. In the case $P=1$ one may determine fixed values considering only the boundaries, i.e. solving $E_{1,0}=0=E_{1,N+1}$, while for $P=2$ this could be obtained from $E_{2,0}=0=E_{2,\lfloor (N+1)/2\rfloor}=E_{2,N+1}$.

Of course, the expressions $E_{P,j}$ contain higher order derivatives. These can be expressed in terms of y and y' by means of the differential equation and y' can be reexpressed in terms of y by means of (fourth-order accurate) finite difference schemes. In this way, the expressions $E_{P,j}$ can be transformed into equations only involving some unknown function values y_p. To cope with this problem, one could first solve the problem with the classical Numerov method.

A NUMERICAL EXAMPLE

To illustrate the methods, we will focus on the particular case where $P=1$. As an example, we consider the problem

$$y'' = \frac{3}{4}y - e^t\,\sin(t/2) \qquad y(0)=1\,, \qquad y(\pi)=0\,,$$

whose solution is given by $y(t) = e^t \cos(t/2)$. Remark that $y(t)$ belongs to the fitting space $\widehat{\mathscr{S}}_{1,1}(1+i/2, 1-i/2)$, but there is no value for μ such that it also belongs to $\mathscr{S}_{1,1}(\mu)$.

For this problem, the lte $E_{1,j}$, after reexpressing the derivatives, becomes

$$E_{1,j} := e^{t_j}\left[\left(-\frac{11}{16}+\frac{3}{2}(\mu_0^2+\mu_1^2)-\mu_0^2\mu_1^2\right)\sin(t_j/2)+\left(\mu_0^2+\mu_1^2-\frac{9}{4}\right)\cos(t_j/2)\right]+\frac{3}{64}(4\mu_0^2-3)(4\mu_1^2-3)\,y(t_j)\,. \tag{3}$$

Substituting $y(t_j) = e^{t_j}\cos(t_j/2)$, $\mu_0 = 1-i/2$ and $\mu_1 = 1+i/2$, one can verify that indeed $E_{1,j} \equiv 0$. Conversely, to determine suitable values for μ_0 and μ_1 in this case, one might try to annihilate the expressions for the lte at the endpoints. Indeed, solving $E_{1,0} = 0 = E_{1,N+1}$ leads to $\{\mu_0^2, \mu_1^2\} = \{3/4-i, 3/4+i\} = \{(1-i/2)^2, (1+i/2)^2\}$. Applying the corresponding EF method, we obtain results that are accurate up to machine accuracy.

Finally, we first apply the classical Numerov method, and then we numerically determine the parameters μ_0^2 and μ_1^2 from locally solving $E_{1,j} = 0 = E_{1,j+1}$ in which $y(t_j)$ and $y(t_{j+1})$ are replaced by the previously obtained values. In that case we obtain a numerical solution that is much more accurate than the previously computed classical solution.

All of this is shown in Figure 1, where we show results that are obtained with $h = 2^{-m}\pi$, $m = 3,4,5,6,7$. The numerical results obtained confirm that the classical Numerov method is a fourth-order method, while the EF-fitted version with numerically computed μ-values behaves like a method of order eight (until machine accuracy is reached).

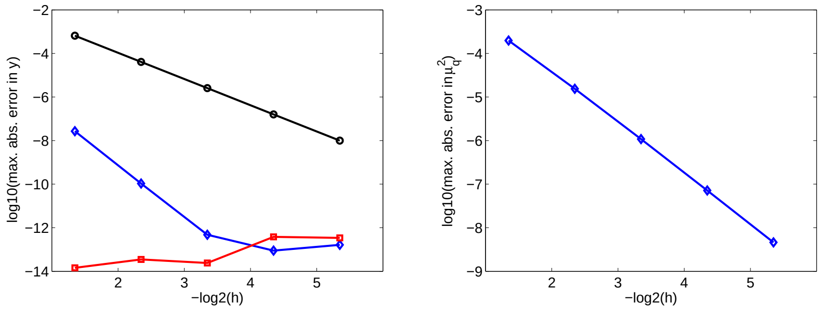

FIGURE 1. Left : $\max_{j\in\{1,\ldots,N\}} |y(t_j) - y_j|$ for the classical method (circles), the EF method with exact values for μ_q^2 (squares) and the EF method with numerically computed values for μ_q^2 (diamonds). For the latter case, the max-norm of the error in μ_q^2 is depicted in the right part of the figure.

CONCLUSION

Second-order boundary value problems are solved by means of a new family of exponentially-fitted variants of the well-known Numerov method. These new methods contain $P+1$ parameters μ_0, μ_1, $\ldots$, μ_P that can be determined either by local arguments of by global arguments and this resp. leads to variable or constant parameter values. In the special case where $\mu_0 = \mu_1 = \ldots = \mu_P = \mu$, a known family of EF methods is obtained. However, in that case the solution is only guaranteed to be real if the parameter value μ is real or purely imaginary. Finally, it is shown how the new EF methods can be used in practice in order to obtain results that are much more accurate than those obtained by the classical Numerov method.

REFERENCES

1. L. Gr. Ixaru and G. Vanden Berghe, *Exponential fitting*, (Kluwer Academic Publishers, Dordrecht, 2004).
2. J.P. Coleman, L.Gr. Ixaru, Truncation errors in exponential fitting for oscillatory problems, *SINUM* **44** (2006) 1441–1465.
3. A. Ghizzetti and A. Ossicini, *Quadrature formulae*, (Birkhaüser, 1970, Basel).
4. D. Hollevoet, M. Van Daele and G. Vanden Berghe, On the leading error term of exponentially fitted Numerov methods, Proceedings of International Conference on Numerical Analysis and Applied Mathematics 2008, eds. T. Simos, G. Psihoyios and C. Tsitouras, American Institute of Physics Conference Proceedings 1048 (2008) 884–887.
5. D. Hollevoet, M. Van Daele and G. Vanden Berghe, *The optimal exponentially-fitted Numerov method for solving two-point boundary value problems*, J. Comp. Appl. Math. 230 (2009) 260–269.